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A Useful Approximation to the Cooling Coefficient of Trace Elements

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ABSTRACT

Radiative cooling is an important ingredient in hydrodynamical models involving evolution of high temperature plasmas. Unfortunately, calculating an accurate cooling coefficient generally requires the solution of over a hundred differential equations to follow the ionization. We discuss here a simple 2-parameter approximation for the cooling coefficient due to elements heavier than H and He, for the temperature range $T = 10^4 - 10^8$ K. Tests of the method show that it successfully tracks the ionization level in severe dynamical environments, and accurately approximates the non-equilibrium cooling coefficient of the trace elements, usually to within 10% in all cases for which cooling is actually important. The error is large only when the temperature is dropping so rapidly due to expansion that radiative cooling is negligible, but even in this situation, the ionization level is followed sufficiently accurately. The current approximation is fully implemented in publicly available FORTRAN code. A second paper will discuss general approaches to approximation methods of this type, other realizations which could be even more accurate, and the potential for extension to calculations of non-equilibrium spectra.

Subject headings: atomic data — radiation mechanisms:thermal — plasmas — hydrodynamics — supernova remnants — ISM:general

1. Introduction

In this paper we present a reliable but compact approximation to the high temperature cooling coefficient of heavy elements in diffuse plasmas under non-equilibrium conditions.² Such an

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²A set of FORTRAN routines to implement this approximation are provided at <ftp://wisp5.physics.wisc.edu/pub/benjamin/BBC>. Documentation is given in the file README.bbc.

approximation is essential for use with multi-dimensional hydrodynamics codes where the additional burden of following the details of ionization evolution severely restricts the available spatial resolution.

With only a few exceptions, large hydrodynamic models that incorporate radiative cooling characterize the cooling coefficient with a single parameter, the temperature, $L(T_e)$, where the total emissivity per unit volume is $\Lambda(T_e) = n_e n_H L(T_e)$ (ergs s⁻¹ cm⁻³) and n_e and n_H are the electron and hydrogen densities. These cooling functions are determined by assuming either that the ionization state at a given temperature is characterized by collisional equilibrium, or that all gas follows a particular pre-calculated ionization history (Shapiro & Moore 1976; Edgar & Chevalier 1983; Sutherland & Dopita 1993).

Because the cooling of a plasma depends on the ionization history of the constituent ions, there can actually be a large range in the value of L at a given T_e , depending upon the details of the ionization evolution. We demonstrate, however, that cooling due to trace elements (those heavier than helium) can be approximated by following the evolution of just a single additional parameter, the mean charge on the trace ions, $\bar{z} = (\sum_{Z,z} A_Z z c_{Z,z}) / \sum_Z A_Z$. Here, Z is the element number, z is the ionic charge, A_Z is the (linear) abundance of element Z relative to hydrogen, and $c_{Z,z} = n_{Z,z} / n_Z$ is the concentration of a given ion (the fraction of element Z with charge z). Because the abundance is dominated by oxygen, \bar{z} ranges from zero to about nine.

Our method generalizes from a cooling curve, $L(T_e)$, to a cooling plane $L(T_e, \bar{z})$. It consequently requires another function that allows us to update the ionization level, $D(T_e, \bar{z}) = (1/n_e)(d\bar{z}/dt)$. With the mean charge as our ionization level indicator, $D(T_e, \bar{z})$ is the difference between the mean ionization and recombination functions. Thus $D(T_e, \bar{z}) = I(T_e, \bar{z}) - R(T_e, \bar{z})$, where $I(T_e, \bar{z}) = (\sum_{Z,z} A_Z i_{Z,z}(T_e) c_{Z,z}) / \sum_Z A_Z$ and $R(T_e, \bar{z}) = (\sum_{Z,z} A_Z r_{Z,z}(T_e) c_{Z,z}) / \sum_Z A_Z$, and where $i_{Z,z}(T_e)$ and $r_{Z,z}(T_e)$ are the ionization and recombination rate coefficients, respectively, at T_e for stage z of element Z . The corresponding cooling coefficient is $L(T_e, \bar{z}) = \sum_{Z,z} A_Z j_{Z,z}(T_e) c_{Z,z}$, where $j_{Z,z}(T_e)$ is the cooling coefficient per ion Z, z .

To implement this approximation we search for a reasonable description of the nonequilibrium ionization concentrations, $c_{Z,z}(T_e, \bar{z})$, representative of those found at T_e and \bar{z} . This assumes that under actual nonequilibrium conditions, the distribution over ion states will depend less on the details of the past history than on how far the present mean charge differs from the collisional equilibrium value at the current temperature. In this paper, we consider the ionization distributions that arise in isothermal relaxation to equilibrium for each temperature T_e , starting with nearly fully ionized or fully neutral gas.

The atomic data used to develop the manifolds comes from Raymond & Smith (1977), with updates described in Raymond & Cox (1985), corrections in oscillator strengths in the cooling transitions of Li-like ions (Shull & Slavin 1994), and revised dielectronic recombination rates of Romanik (1988). The abundances are taken from Anders & Grevesse (1989). The effects of charge exchange are not included; errors introduced by neglecting this are smaller than the uncertainties

in the atomic data and elemental abundances used to generate the cooling curve.

2. A Manifold of Isothermal Evolutions

We have performed the manifold of non-equilibrium isothermal evolutions described below to form the basis for our approximation, producing tables of the cooling coefficient of trace elements $L(T_e, \bar{z})$ and our ionization evolution functions $I(T_e, \bar{z})$ and $R(T_e, \bar{z})$.

Gas is initialized with equilibrium ionization appropriate to some initial temperature T_o . Its temperature is then suddenly changed to T_e and held fixed as the ionization evolves to equilibrium. By choosing T_o to be low (e.g., $10^{4.0}$ K), and performing the calculation for a dense set of temperatures T_e between $10^{4.0}$ and $10^{8.0}$ K, the runs sample the full range of conditions possible in under-ionized gases. By repeating the whole set once again with very high T_o (e.g. $10^{8.0}$ K), conditions representing over-ionized gases are explored. Together these cases sample the full range of \bar{z} .

A particular moment in an evolution can be characterized by T_o , T_e , and the fluence ($f = \int n_e dt$). The ionization state is known, allowing straightforward evaluation of the mean charge \bar{z} and then using \bar{z} as the index of the time evolution. Evolution at constant temperature makes it easy to acquire the tables of $L(T_e, \bar{z})$, $I(T_e, \bar{z})$, $R(T_e, \bar{z})$, and $D(T_e, \bar{z})$ on a fixed grid of T_e and \bar{z} .

The cooling function shown in Figure 1 shows a huge peak at $T_e \sim 10^6$ K and $\bar{z} \sim 2$ due to collisional excitation of low stages of ionization. It falls rapidly to the left due to Boltzmann factors, and gradually to the right due to decreasing excitation cross-sections. It falls at higher \bar{z} as fewer bound electrons with low enough energy are available for collisional excitation. Above the equilibrium line the gas is over-ionized and collisional excitation is difficult, particularly at lower temperatures. At a given \bar{z} , the mean ionization function, I , behaves much like the collisionally excited cooling, with vagaries at the transition from $\bar{z} = 1$ to 2, and at $\bar{z} \cong 6$ where the mean ionization rate is sensitive to the relative proportions of helium- and lithium-like oxygen.

The structure of the mean recombination rate, R , is more gradual. In the upper left corner it is dominated by radiative recombination and the gradual increase with \bar{z} and decrease with temperature are as expected. Deviations from that smooth pattern in the rest of the diagram are due to dielectronic recombination. In both I and R , there are distortions in the patterns just above the equilibrium line. These arise because, in relaxing to equilibrium, a recombining plasma goes through a considerable compaction of its ionization distribution.

The principal feature of the rate function $D(\bar{z}, T_e)$ is that ionization toward equilibrium from below is much faster than recombination toward it from above. With increasing distance from equilibrium, the ionization rate increases dramatically, the recombination rate only gradually.

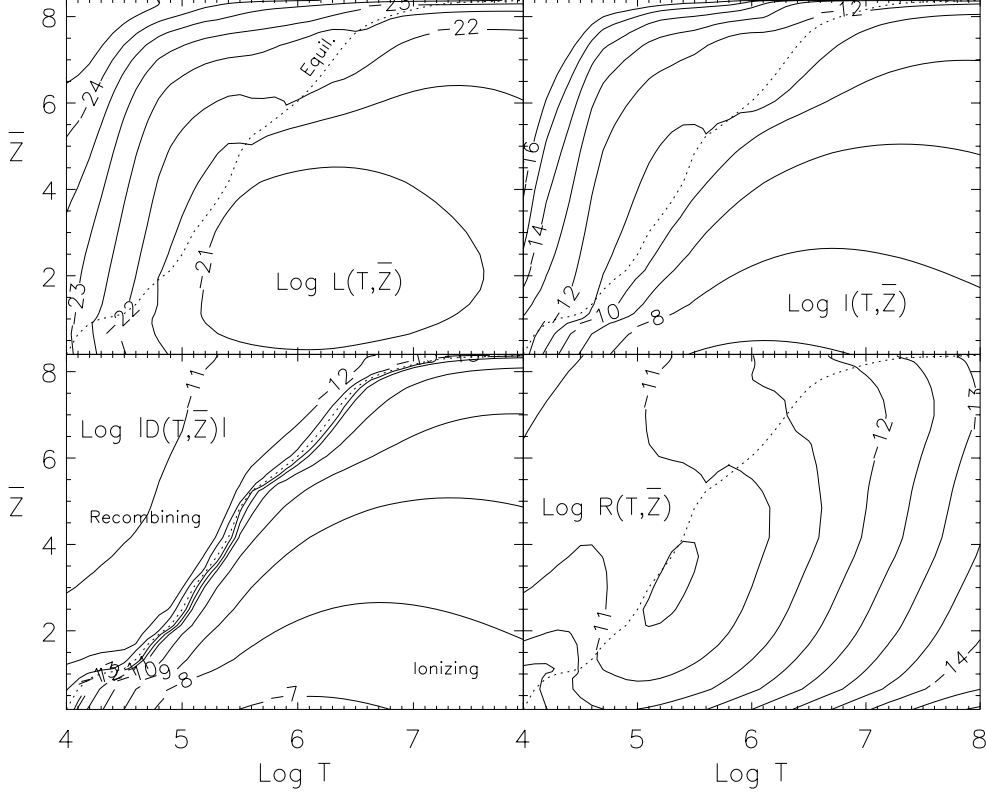


Fig. 1.— Contours of the trace element cooling coefficient, $L(T_e, \bar{z})$ (erg cm³ s⁻¹) [top left panel], the mean ionization rate coefficient, $I(T_e, \bar{z})$ (cm³ s⁻¹) [top right panel], the mean recombination rate coefficient, $R(T_e, \bar{z})$ (cm³ s⁻¹) [bottom right panel], and the absolute value of the ionization evolution function, $|D(\bar{z}, T_e)|$ (cm³ s⁻¹) [bottom left panel], as a function of electron temperature and mean charge \bar{z} . The dotted line in each panel shows the mean charge in collisional equilibrium as a function of gas temperature, $z_{eq}(T_e)$. The function $|D(\bar{z}, T_e)|$ (cm³ s⁻¹) passes through zero along this line. Above the equilibrium curve, the gas is recombining and $D(\bar{z}, T_e)$ is negative; below, it is ionizing and $D(\bar{z}, T_e)$ is positive. These functions were calculated for a grid of isothermal evolutions. Gas was either started with ionization fractions corresponding to $T_o = 10^4$ K or $T_o = 10^8$ K. It then ionized up or recombined down to $\bar{z}_{eq}(T_e)$ at fixed temperature T_e . The resultant rate coefficients were calculated versus \bar{z} for each T_e for the range $T_e = 10^4 - 10^8$ K.

3. Testing With Cooling Blast Wave Evolutions

To test the accuracy of our approximation for a wide range of situations, a representative set of cases were examined in which single parcels of gas in collisional equilibrium at 10^4 K were suddenly shock heated and then subjected to varying degrees of expansion. The test situation was modeled on the Sedov blast wave solution for an explosion of energy 10^{51} ergs into a homogeneous medium

of particle density n_o . By varying the preshock density and the assumed distance of the parcel from the explosion site, we adjusted the post shock temperature and the timescales for depressurization versus radiative cooling. These scenarios test the two behaviors in which drastic departures from equilibrium occur: the rapid ionization of gas passing through a shock front and the rapid adiabatic cooling of an over-ionized plasma.

Each parcel’s evolution can be fully characterized by n_o and T_2 . We have approximated $p(t) = p_2(t_2/t)^\alpha$, with t_2 being the time the parcel is shocked, and $\alpha = 1.9$ determining the rate of decompression. The temperature evolution is then

$$\frac{dT}{dt} = -\frac{2}{5}T \left(\frac{L(T, \bar{z})n_en_H}{p} + \frac{\alpha}{t} \right). \quad (1)$$

where n_H is the particle density of hydrogen (ionized and neutral).

We have carried out each simulation twice, first, solving the full ionization balance evolution exactly, then using our cooling approximation. In the latter, we solve the ionization evolution for hydrogen, helium, and \bar{z} (four rate equations). The cooling is the sum of that from hydrogen, helium, and our tabulated cooling function.

In order to test the widest possible range of conditions, we chose three values of T_2 , with three different values of n_o for each. The values of density were spaced to alter the initial ratio of depressurization to radiative cooling from approximately 0.4 at the high density end, to 6 and then 4000 at the lower densities. For the densest runs, the structure is very similar to that of a steady state radiative shock. For the next lower density cases, depressurization has strong effects but cooling is still sufficiently rapid that the density eventually rises rather than falling with time. At the lowest densities, the density and temperature fall adiabatically and the ionization level is soon frozen in.

Figure 2 shows the exact trace element cooling coefficient evolutions versus temperature, the ratio of our approximate results to the exact ones, and the evolutions of mean charge, both exact and approximate. In each case, the cooling function begins very high just after the shock, when the gas is still briefly nearly neutral. At the two higher temperatures in the middle and right hand panels, the gas rapidly ionizes up and the cooling function drops precipitously to very close to the equilibrium value. This “ion flash” is so rapid that the integrated cooling during this period is negligible, as evidenced by the nearly vertical tracks. Thereafter, these tracks follow the equilibrium curve down to just below 10^6K , after which their recombination cannot keep up with the cooling and the cooling rate falls below the equilibrium value. In the lowest temperature cases, significant cooling takes place before the cooling function drops through equilibrium, after which it plunges toward the nonequilibrium curve of the initially higher temperature cases. The differences between the radiation dominated and mixed evolutions are almost negligible. In the expansion dominated cases, however, things are quite different. The temperature drops so rapidly that the gas is soon over-ionized; recombination is slower than the temperature drop, and the ionization level declines

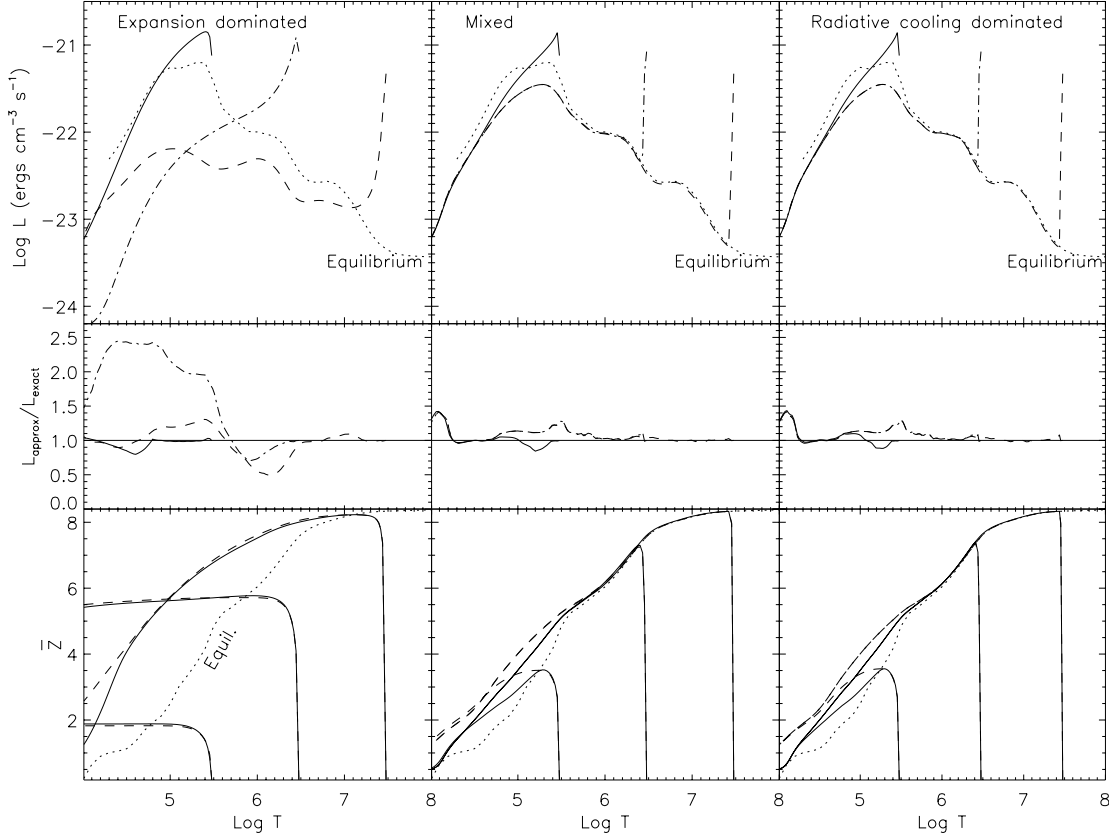


Fig. 2.— Comparison of cooling and ionization evolution for nine cases using the full ionization evolution and the approximation presented in this paper. The top row shows the evolution of the exact trace element cooling coefficient versus temperature. The left panel shows expansion-dominated evolution with $(n_o, T_2) = (1 \text{ cm}^{-3}, 3 \times 10^7 \text{ K})$ (dashed), $(3 \times 10^{-4} \text{ cm}^{-3}, 3 \times 10^6 \text{ K})$ (dash-dot), and $(10^{-7} \text{ cm}^{-3}, 3 \times 10^5 \text{ K})$ (solid); the central panel shows “mixed” evolution with $(n_o, T_2) = (2 \times 10^4 \text{ cm}^{-3}, 3 \times 10^7 \text{ K})$ (dashed), $(10 \text{ cm}^{-3}, 3 \times 10^6 \text{ K})$ (dash-dot), and $(2 \times 10^{-3} \text{ cm}^{-3}, 3 \times 10^5 \text{ K})$ (solid); the right panel shows radiative cooling dominated evolution with $(n_o, T_2) = (10^6 \text{ cm}^{-3}, 3 \times 10^7 \text{ K})$ (dashed), $(300 \text{ cm}^{-3}, 3 \times 10^6 \text{ K})$ (dash-dot), and $(0.1 \text{ cm}^{-3}, 3 \times 10^5 \text{ K})$ (solid). The time evolution for each curve is from right to left. The cooling curve for collisional ionization equilibrium is also shown (dotted). The middle set of panels shows the ratio of the approximation for trace element cooling to the exact value for each of the above cases. For “mixed” and “radiative” evolution, the highest temperature cases are sufficiently similar that the curves overlie each other. The lowest set of panels show the ionization evolution for these cases in the T - z plane. The solid curves show the exact evolution for the nine cases above, while the dashed lines show the slight departures that result by using the approximation we present. The dotted line in each panel shows the mean charge in collisional equilibrium as a function of gas temperature, $z_{eq}(T_e)$, as in Figure 1.

only gradually or is frozen in.

The middle row of panels shows the ratio of approximate to exact cooling coefficients. In the two right hand panels, the approximation is good to within about 10% except below $10^{4.2}\text{K}$ where it is consistently high by about 40%, and in a peak at $10^{5.5}\text{K}$ where it can be as much as 20 to 30% high. At this temperature, the approximate \bar{z} evolutions of the two higher temperature cases in the two right lower panels of Figure 2 diverge by +0.4 charge states from the exact results. This is due in part to the excess cooling, but the recombination rate is almost certainly slightly too low as well.

For the rapidly depressurizing cases, radiative cooling is inconsequential. Nevertheless, the cooling coefficient which differs substantially from the other cases, is still reasonably well fit, except for the intermediate temperature case for which \bar{z} gets frozen at a value of 5.5. In that case, the value of \bar{z} is well represented by the approximation, but the approximate cooling coefficient is too high. The freezing in of the ionization is extremely well matched, except very late in the highest initial temperature case.

We have also compared the time evolution of density, temperature, mean charge, and the cooling coefficients for the exact calculation, our approximation, and the case where the trace elements are assumed to be in collisional ionization equilibrium. While the time evolution of temperature and density of the exact calculations and our approximation are in reasonably good agreement, the case with collisional ionization equilibrium shows significant differences in the time evolution of temperature. In addition, the ionization equilibrium assumption provides a poor estimate of the true ionization level of the gas, especially for the expansion dominated cases.

4. Summary and Conclusions

We provide a means by which large hydrocodes can include an accurate approximation to the radiative cooling coefficient, one far more responsive to the vagaries of dynamical environments than any single function of temperature. The method also follows the mean ionization level of the gas. Both the trace element cooling coefficient $L(T_e, \bar{z})$, and the rate of change of \bar{z} depend only on the identification of a manifold of representative ionization concentrations found at a particular temperature and mean charge. The ionization concentrations we used came from the isothermal relaxations of both highly over-ionized and highly under-ionized gas. In the test cases presented, both the cooling coefficient and mean charge evolution are quite accurately approximated. For all cases in which radiative cooling is significant, the approximation never errs by more than 30%. The error is usually less than 10 to 15%, well within the accuracy of the true cooling coefficient, which is limited by uncertainties in atomic data and abundances. The error in the cooling coefficient can be somewhat larger in examples with extreme amounts of depressurization, but never by enough to make the negligible radiative cooling appear to be significant.

Our approximate cooling coefficients and charge evolution rates, however, showed patterns

in their modest errors, patterns which we believe we understand and can eliminate with future work. Should a potential user wait for these improvements before beginning to implement this method? The current model provides an excellent approximation for the cooling coefficient. If one is interested only in dynamics, it is certainly sufficient. Implementation of the next generation requires only swapping one set of tables for another. Our future work will also examine the possibility that the ion distributions can be used to provide absorption and emission spectra in post processing. It is possible to do this at the two parameter level, but higher order corrections will also be examined. The latter are expected to be two to four times more complex, and will be pursued only if spectral accuracy requires it.

An additional consideration for gas with $T \sim 10^4$ K and $\bar{z} \lesssim 2$ is the effect of photoionization on the ionization balance and therefore the cooling. Our scheme can be easily modified to incorporate photoionization of hydrogen and helium. However, the effects of photoionization of trace elements would require a table of photoionization correction factors for $L(T_e, \bar{z})$ and $D(T_e, \bar{z})$. This too will be considered in future refinements.

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